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Three-particle correlations in liquid and amorphous aluminium

Bulat N. Galimzyanov*, Anatolii V. Mokshin

Institute of Physics, Kazan Federal University, 420008 Kazan, Russia
Landau Institute for Theoretical Physics, Russian Academy of Sciences, 142432 Chernogolovka, Russia

HIGHLIGHTS

- The original method of three-particle structural analysis is proposed.
- The original three-particle correlation function is introduced.
- The time evolution of three-particle correlations is evaluated for liquid and amorphous aluminium.
- The "stable" disordered structures are detected, that are formed by triplets with various configurations.
- Transitions between the various configurations of triplets are observed.

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ABSTRACT

Analysis of three-particle correlations is performed on the basis of simulation data of atomic dynamics in liquid and amorphous aluminium. A three-particle correlation function is introduced to characterize the relative positions of various three particles—the so-called triplets. Various configurations of triplets are found by calculation of pair and three-particle correlation functions. It was found that in the case of liquid aluminium with temperatures 1000 K, 1500 K, and 2000 K the three-particle correlations are more pronounced within the spatial scales, comparable with a size of the second coordination sphere. In the case of amorphous aluminium with temperatures 50 K, 100 K, and 150 K these correlations in the mutual arrangement of three particles are manifested up to spatial scales, which are comparable with a size of the third coordination sphere. Temporal evolution of three-particle correlations is analyzed by using a time-dependent three-particle correlation function, for which an integro-differential equation of type of the generalized Langevin equation is output with help of projection operators technique. A solution of this equation by means of mode-coupling theory is compared with our simulation results. It was found that this solution correctly reproduces the behavior of the time-dependent three-particle correlation functions for liquid and amorphous aluminium.

1. Introduction

At present time the main attention is paid to study the structure of condensed systems, which are in equilibrium or in metastable states [1–4]. Often, the traditional experimental methods of structural analysis do not allow to correctly identify the presence of some structures in bulk systems due to their small sizes, either low concentrations in the system, or due to relatively short lifetimes. Usually, information about the structure of condensed systems is extracted by using microscopic

* Corresponding author at: Institute of Physics, Kazan Federal University, 420008 Kazan, Russia.
E-mail addresses: bulatgnmail@gmail.com (B.N. Galimzyanov), anatolii.mokshin@mail.ru (A.V. Mokshin).

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